Unless noted, all energies are in Hartrees

1
Gasphase Energy: -232.2531
Solvation Phase Energy: -232.2550
Zero Point Energy: 63.09 kcal/mol
Coordinates:

C	2.5048	-0.0490	-0.0000
C	1.8059	1.1615	-0.0000
C	0.4082	1.1615	0.0000
C	-0.2907	-0.0490	0.0001
C	0.4082	-1.2595	0.0000
C	1.8059	-1.2595	-0.0000
H	3.5911	-0.0490	0.0000
H	2.3491	2.1023	-0.0001
H	-0.1350	2.1023	-0.0002
H	-1.3770	-0.0490	-0.0001
H	-0.1350	-2.2003	-0.0001
H	2.3491	-2.2003	-0.0001

2
Gasphase Energy: -78.5919
Solvation Phase Energy: -78.5933
Zero Point Energy: 32.07 kcal/mol
Coordinates:

C	0.0693	1.1652	0.0000
C	-1.2615	1.1653	-0.0000
H	0.6419	0.2413	0.0000
H	-1.8341	0.2413	0.0000
H	-1.8341	2.0892	0.0000
H	0.6419	2.0892	0.0000

3
Gasphase Energy: -310.8785
Solvation Phase Energy: -310.8804
Zero Point Energy: 98.084
Coordinates:

C	2.5116	-0.0490	0.0000
C	1.8093	1.1674	0.0000
C	0.4048	1.1674	0.0000
C	-0.2974	-0.0490	0.0000
C	0.4048	-1.2654	0.0000
C	1.8094	-1.2654	0.0000
H	3.6150	-0.0490	0.0000

H	2.3611	2.1230	0.0000
H	-0.1469	2.1230	0.0000
H	-0.1469	-2.2209	0.0000
H	2.3611	-2.2210	0.0000
C	-1.8194	-0.0490	0.0000
H	-2.1924	0.4784	0.9136
H	-2.1924	0.4784	-0.9136
C	-2.3281	-1.4877	0.0000
H	-1.9551	-2.0152	-0.9136
H	-1.9551	-2.0152	0.9136
H	-3.4470	-1.4877	0.0000

4
Gasphase Energy: -1966.1779
Solvation Phase Energy: -1966.1976
Zero Point Energy: 290.12 kcal/mol
Coordinates:

Ir	0.9528	-0.1735	0.2752
O	1.8005	-0.0143	2.1497
C	1.1233	-0.1632	3.2012
C	-0.2601	-0.4864	3.3137
C	-1.2042	-0.3878	2.2548
O	-0.9796	-0.2287	1.0213
H	-2.2599	-0.4877	2.5264
H	-0.6749	-0.4184	4.3141
H	1.6871	-0.0768	4.1353
O	0.1024	-0.3484	-1.5773
C	0.8245	-0.3778	-2.6316
C	2.2179	-0.3321	-2.7378
C	3.1209	-0.2223	-1.6742
O	2.8710	-0.1766	-0.4234
H	4.1877	-0.1819	-1.9172
H	2.6362	-0.3591	-3.7375
H	0.2495	-0.4571	-3.5609
C	1.1344	-2.6530	0.2862
Ir	-0.0657	-2.9634	3.3309
O	-1.9785	-2.9614	4.0411
O	1.8630	-2.9087	2.5755
O	0.7946	-2.7815	5.1781
O	-0.9210	-3.1272	1.4596
C	2.0827	-2.7512	1.3410
C	-0.2483	-2.9772	0.4052
C	0.0790	-2.7500	6.2368
C	-1.3136	-2.7983	6.3514
C	-2.2219	-2.9129	5.2930

H	3.1373	-2.6522	1.0652
H	-0.8163	-3.0643	-0.5263
H	0.6596	-2.6665	7.1623
H	-1.7262	-2.7690	7.3534
H	-3.2873	-2.9549	5.5416
H	1.5443	-2.7209	-0.7161
C	0.0472	-5.0878	3.5768
H	0.4674	-5.2011	4.5792
C	0.8424	1.9519	0.0371
H	0.4222	2.0695	-0.9647
C	-1.3450	-5.7034	3.6298
O	-1.8070	-6.0017	4.7223
C	1.0016	-5.6520	2.5511
O	0.7249	-5.7841	1.3652
C	-0.1105	2.5156	1.0648
O	0.1661	2.6423	2.2512
C	2.2358	2.5650	-0.0140
O	2.6982	2.8652	-1.1058
C	-2.1427	-5.9152	2.3627
H	-1.5368	-6.3869	1.5863
H	-3.0251	-6.5121	2.6001
H	-2.4499	-4.9404	1.9712
C	2.3666	-6.0559	3.0825
H	2.8248	-5.2179	3.6179
H	2.2567	-6.8780	3.7999
H	3.0075	-6.3740	2.2582
C	-1.4737	2.9271	0.5345
H	-1.9353	2.0932	-0.0043
H	-2.1135	3.2447	1.3599
H	-1.3603	3.7515	-0.1798
C	3.0337	2.7717	1.2537
H	2.4294	3.2453	2.0302
H	3.3363	1.7953	1.6445
H	3.9187	3.3653	1.0175

5
Gasphase Energy: -1059.5191
Solvation Phase Energy: -1059.5359
Zero Point Energy: 160.20 kcal/mol
Coordinates:

Ir	0.0338	0.4137	0.3583
O	2.3600	0.5560	0.6195
H	2.6680	1.0023	-0.1825
H	2.4823	1.1852	1.3453
O	0.0357	-0.7649	2.0320

C	0.2481	-2.0215	1.9640
C	0.5170	-2.8024	0.8360
C	0.5627	-2.3419	-0.4810
O	0.3833	-1.1538	-0.9180
H	0.7780	-3.0757	-1.2660
H	0.6787	-3.8624	0.9956
H	0.2242	-2.5289	2.9349
O	0.1877	1.6061	-1.3081
C	0.0309	2.8735	-1.2323
C	-0.1947	3.6583	-0.0981
C	-0.2694	3.1953	1.2221
O	-0.1499	1.9996	1.6508
H	-0.4285	3.9400	2.0093
H	-0.3195	4.7241	-0.2532
H	0.0991	3.3899	-2.1971
C	-2.0599	0.3998	0.0634
H	-2.2148	1.1627	-0.7052
C	-2.8110	0.9022	1.2919
O	-3.2467	2.0455	1.2783
C	-2.4688	-0.9506	-0.4862
O	-2.6834	-1.9338	0.2086
C	-2.9925	0.0151	2.5020
H	-3.3084	-0.9877	2.2070
H	-2.0258	-0.0923	3.0046
H	-3.7095	0.4840	3.1785
C	-2.6071	-1.0184	-1.9990
H	-3.4728	-0.4217	-2.3121
H	-1.7225	-0.5947	-2.4832
H	-2.7517	-2.0543	-2.3115

6
Gasphase Energy: -1117.8506
Solvation Phase Energy: -1231.4164
Zero Point Energy: 187.43 kcal/mol
Coordinates:

Ir	0.0595	0.4275	0.3842
O	0.0058	-0.7879	2.0408
C	0.2231	-2.0409	1.9453
C	0.5454	-2.7908	0.8085
C	0.6133	-2.3099	-0.5013
O	0.4386	-1.1173	-0.9254
H	0.8424	-3.0345	-1.2915
H	0.7019	-3.8543	0.9503
H	0.1562	-2.5788	2.8980
O	0.1993	1.6384	-1.2673

C	0.0458	2.9028	-1.1597
C	-0.1980	3.6613	-0.0119
C	-0.3157	3.1717	1.2955
O	-0.2106	1.9700	1.7068
H	-0.5088	3.9004	2.0900
H	-0.3190	4.7303	-0.1472
H	0.1238	3.4428	-2.1109
C	-2.0725	0.3686	0.0440
H	-2.2169	1.1235	-0.7340
C	-2.8414	0.8671	1.2518
O	-3.2534	2.0211	1.2569
C	-2.4392	-0.9843	-0.5008
O	-2.6440	-1.9776	0.1873
C	-3.0690	-0.0351	2.4460
H	-3.4101	-1.0240	2.1323
H	-2.1139	-0.1805	2.9609
H	-3.7816	0.4452	3.1195
C	-2.5500	-1.0633	-2.0182
H	-3.4379	-0.5082	-2.3456
H	-1.6796	-0.6016	-2.4932
H	-2.6446	-2.1058	-2.3289
C	4.9627	0.8793	1.0398
C	4.4329	0.6752	-0.2355
C	3.0550	0.5431	-0.3801
N	2.2181	0.6052	0.6734
C	2.7238	0.8018	1.9061
C	4.0907	0.9436	2.1279
H	6.0337	0.9868	1.1827
H	5.0721	0.6189	-1.1103
H	2.5835	0.3840	-1.3438
H	1.9966	0.8431	2.7096
H	4.4567	1.1012	3.1368

7
Gasphase Energy: -945.9718
Solvation Phase Energy: -945.9848
Zero Point Energy: 146.08 kcal/mol
Coordinates:

Ir	0.1498	0.4534	0.2919
O	2.5200	0.6845	0.5648
H	2.8034	1.1504	-0.2346
H	2.5846	1.3273	1.2857
O	0.1149	-0.7229	1.9633
C	0.2015	-1.9924	1.8748
C	0.3617	-2.7802	0.7298

C	0.4881	-2.3060	-0.5805
O	0.4608	-1.1014	-0.9988
H	0.6421	-3.0493	-1.3718
H	0.4128	-3.8539	0.8727
H	0.1515	-2.5110	2.8394
O	0.2841	1.6547	-1.3715
C	0.0815	2.9119	-1.2933
C	-0.1600	3.6889	-0.1536
C	-0.2020	3.2238	1.1660
O	-0.0586	2.0301	1.5950
H	-0.3603	3.9683	1.9556
H	-0.3090	4.7523	-0.3056
H	0.1248	3.4343	-2.2567
C	-1.8423	0.2990	0.0738
C	-2.4149	0.0926	-1.1929
C	-3.8017	-0.0045	-1.3438
C	-4.6435	0.1016	-0.2343
C	-4.0845	0.3041	1.0297
C	-2.6981	0.4015	1.1839
H	-2.2766	0.5576	2.1724
H	-4.7278	0.3865	1.9029
H	-5.7212	0.0261	-0.3528
H	-4.2229	-0.1641	-2.3339
H	-1.7719	0.0075	-2.0639

7 optimized in solvent (benzene)
Solvation Phase Energy: -945.9850
Zero Point Energy: 146.29 kcal/mol

Ir	0.1514	0.4577	0.2937
O	2.5039	0.6886	0.5500
H	2.8584	1.0947	-0.2544
H	2.6674	1.3270	1.2605
O	0.1144	-0.7270	1.9649
C	0.2001	-1.9981	1.8771
C	0.3624	-2.7843	0.7308
C	0.4927	-2.3104	-0.5792
O	0.4687	-1.1028	-0.9952
H	0.6463	-3.0532	-1.3709
H	0.4124	-3.8587	0.8732
H	0.1465	-2.5183	2.8408
O	0.2763	1.6574	-1.3694
C	0.0839	2.9183	-1.2929
C	-0.1547	3.6955	-0.1532
C	-0.2040	3.2303	1.1661
O	-0.0732	2.0332	1.5932
H	-0.3591	3.9743	1.9565

H -0.2909 4.7612 -0.3043
H 0.1308 3.4390 -2.2567
C -1.8397 0.2897 0.0749
C -2.4140 0.0853 -1.1928
C -3.8005 -0.0142 -1.3486
C -4.6464 0.0874 -0.2407
C -4.0889 0.2879 1.0253
C -2.7022 0.3873 1.1814
H -2.2850 0.5428 2.1719
H -4.7338 0.3676 1.8981
H -5.7241 0.0111 -0.3620
H -4.2187 -0.1714 -2.3409
H -1.7704 0.0044 -2.0639

8
Gasphase Energy: -1117.8506
Solvation Phase Energy: -1117.8605
Zero Point Energy: 187.43 kcal/mol
Coordinates:
O 1.5779 -0.4952 1.3880
C 1.3080 -0.4648 2.6332
C 0.0621 -0.5706 3.2639
C -1.1743 -0.7508 2.6321
O -1.4290 -0.8409 1.3863
H -2.0572 -0.8383 3.2771
H 0.0553 -0.5161 4.3471
H 2.1868 -0.3495 3.2793
O -1.4282 -0.8408 -1.3860
C -1.1727 -0.7511 -2.6318
C 0.0644 -0.5716 -3.2627
C 1.3097 -0.4665 -2.6312
O 1.5789 -0.4967 -1.3860
H 2.1889 -0.3516 -3.2768
H 0.0583 -0.5174 -4.3460
H -2.0553 -0.8385 -3.2773
C -0.1571 1.3761 -0.0005
C -1.4346 1.9652 0.0027
C -1.5928 3.3548 0.0020
C -0.4745 4.1924 -0.0022
C 0.8021 3.6246 -0.0053
C 0.9572 2.2348 -0.0044
H 1.9572 1.8095 -0.0067
H 1.6819 4.2647 -0.0085
H -0.5963 5.2727 -0.0028
H -2.5931 3.7830 0.0048
H -2.3150 1.3278 0.0060

Ir	0.0722	-0.6437	0.0006
C	0.6414	-5.6530	-0.0058
C	-0.6326	-5.0819	-0.0060
C	-0.7472	-3.6941	-0.0023
N	0.3280	-2.8852	0.0017
C	1.5568	-3.4331	0.0019
C	1.7553	-4.8115	-0.0016
H	0.7635	-6.7321	-0.0089
H	-1.5269	-5.6964	-0.0092
H	-1.7097	-3.1926	-0.0022
H	2.3828	-2.7293	0.0052
H	2.7642	-5.2106	-0.0012

9
Gasphase Energy: -948.1427
Solvation Phase Energy: -948.1501
Zero Point Energy: 165.12 kcal/mol
Coordinates:

Ir	-0.3047	0.0644	-0.1711
O	-1.9760	-0.1055	-1.3686
O	0.8108	0.2582	-1.9139
C	2.0791	0.3629	-1.8666
C	2.9197	0.3693	-0.7478
C	2.5138	0.2637	0.5854
O	1.3333	0.1622	1.0590
H	3.2980	0.2713	1.3513
H	3.9843	0.4601	-0.9315
H	2.5575	0.4549	-2.8494
C	-0.4410	2.1316	-0.2479
C	-1.1203	2.7369	-1.3158
C	-1.1444	4.1286	-1.4563
C	-0.4920	4.9463	-0.5317
C	0.1866	4.3564	0.5364
C	0.2089	2.9651	0.6764
H	0.7424	2.5297	1.5165
H	0.7012	4.9770	1.2664
H	-0.5119	6.0272	-0.6415
H	-1.6778	4.5717	-2.2941
H	-1.6343	2.1186	-2.0437
O	0.2174	-2.0612	-0.4638
C	-0.4674	-2.7763	-1.2484
C	-2.2715	-1.1930	-1.9734
C	-1.6331	-2.4336	-1.9600
H	-0.1039	-3.8067	-1.3829
H	-3.1746	-1.1120	-2.5908

H -2.0779 -3.2113 -2.5716
C -1.6217 0.5147 1.5474
C -1.3989 -0.8606 1.4839
H -1.0667 1.1293 2.2466
H -0.6534 -1.3276 2.1196
H -2.1426 -1.5235 1.0517
H -2.5349 0.9487 1.1551

10
Gasphase Energy: -869.5276
Solvation Phase Energy: -869.5412
Zero Point Energy: 130.49 kcal/mol
Coordinates:
Ir 0.0680 -0.6211 0.0084
O 1.5630 -0.5280 1.3942
C 1.3089 -0.5427 2.6455
C 0.0679 -0.6592 3.2811
C -1.1661 -0.8229 2.6427
O -1.4129 -0.8663 1.3908
H -2.0514 -0.9456 3.2771
H 0.0656 -0.6500 4.3654
H 2.1974 -0.4656 3.2826
O -1.4116 -0.8657 -1.3732
C -1.1669 -0.8107 -2.6252
C 0.0652 -0.6374 -3.2646
C 1.3071 -0.5259 -2.6299
O 1.5629 -0.5240 -1.3789
H 2.1945 -0.4418 -3.2677
H 0.0607 -0.6170 -4.3488
H -2.0529 -0.9308 -3.2593
C -0.1583 1.3703 0.0028
C -1.4422 1.9333 -0.0017
C -1.5923 3.3242 -0.0090
C -0.4725 4.1590 -0.0118
C 0.8050 3.5943 -0.0072
C 0.9681 2.2050 0.0000
H 1.9629 1.7728 0.0028
H 1.6846 4.2333 -0.0094
H -0.5941 5.2386 -0.0175
H -2.5920 3.7516 -0.0127
H -2.3161 1.2907 -0.0002

11
Gasphase Energy: -948.1368

Solvation Phase Energy: -948.1452
Zero Point Energy: 164.62 kcal/mol
Coordinates:

Ir	0.0584	-0.5500	0.0001
O	1.6243	-0.2915	1.3237
C	1.4010	-0.1756	2.5722
C	0.1866	-0.2830	3.2617
C	-1.0694	-0.5286	2.6931
O	-1.3722	-0.7012	1.4672
H	-1.9241	-0.5939	3.3771
H	0.2211	-0.1578	4.3384
H	2.2992	0.0228	3.1693
O	-1.5274	-0.6167	-1.3233
C	-1.3330	-0.4575	-2.5719
C	-0.1223	-0.3145	-3.2617
C	1.1573	-0.2991	-2.6932
O	1.4892	-0.4071	-1.4674
H	2.0073	-0.1884	-3.3773
H	-0.1818	-0.1985	-4.3383
H	-2.2529	-0.4465	-3.1687
C	-0.1502	1.4756	-0.0000
C	-1.4195	2.0675	0.1009
C	-1.5624	3.4587	0.0997
C	-0.4394	4.2834	0.0000
C	0.8282	3.7048	-0.0997
C	0.9718	2.3138	-0.1010
H	1.9624	1.8759	-0.1790
H	1.7105	4.3360	-0.1781
H	-0.5507	5.3646	0.0001
H	-2.5549	3.8967	0.1781
H	-2.3001	1.4370	0.1789
C	-0.0710	-2.9843	-0.5642
C	0.6816	-2.9070	0.5628
H	-1.1427	-3.1452	-0.5188
H	0.3868	-3.0007	-1.5479
H	0.2370	-3.0175	1.5465
H	1.7636	-2.8455	0.5174

12
Gasphase Energy: -948.0629
Solvation Phase Energy: -948.0736
Zero Point Energy: 162.62 kcal/mol
Coordinates:

Ir	-0.2280	-0.1531	0.1092
O	1.3085	1.6915	4.0718

C	2.4261	1.1913	3.9984
C	2.9265	0.2973	2.9663
C	2.2173	-0.1249	1.8750
O	0.9735	0.2154	1.6587
H	2.6928	-0.7861	1.1465
H	3.9494	-0.0549	3.0644
H	3.1816	1.4247	4.7851
O	1.0181	0.3334	-1.3979
C	0.6530	0.2979	-2.6291
C	-0.5799	-0.0325	-3.1760
C	-1.7161	-0.4046	-2.4359
O	-1.8222	-0.4960	-1.1761
H	-2.6313	-0.6353	-2.9941
H	-0.6710	0.0020	-4.2554
H	1.4611	0.5862	-3.3096
C	0.3152	-2.0913	-0.1270
C	1.5652	-2.5365	-0.5826
C	1.8739	-3.8989	-0.6004
C	0.9372	-4.8412	-0.1643
C	-0.3171	-4.4124	0.2735
C	-0.6323	-3.0486	0.2723
H	-1.6282	-2.7360	0.5825
H	-1.0597	-5.1351	0.6018
H	1.1802	-5.8999	-0.1748
H	2.8507	-4.2242	-0.9500
H	2.3052	-1.8170	-0.9230
C	-0.7611	2.2344	0.0902
C	-1.3973	1.6627	1.1568
H	0.2231	2.6767	0.2045
H	-1.2722	2.4002	-0.8533
H	-0.9214	1.6524	2.1343
H	-2.4438	1.3759	1.0874

13
Gasphase Energy: -869.4930
Solvation Phase Energy: -869.5097
Zero Point Energy: 130.13 kcal/mol
Coordinates:

Ir	-0.2280	-0.1531	0.1092
O	1.3085	1.6915	4.0718
C	2.4261	1.1913	3.9984
C	2.9265	0.2973	2.9663
C	2.2173	-0.1249	1.8750
O	0.9735	0.2154	1.6587
H	2.6928	-0.7861	1.1465

H	3.9494	-0.0549	3.0644
H	3.1816	1.4247	4.7851
O	1.0181	0.3334	-1.3979
C	0.6530	0.2979	-2.6291
C	-0.5799	-0.0325	-3.1760
C	-1.7161	-0.4046	-2.4359
O	-1.8222	-0.4960	-1.1761
H	-2.6313	-0.6353	-2.9941
H	-0.6710	0.0020	-4.2554
H	1.4611	0.5862	-3.3096
C	0.3152	-2.0913	-0.1270
C	1.5652	-2.5365	-0.5826
C	1.8739	-3.8989	-0.6004
C	0.9372	-4.8412	-0.1643
C	-0.3171	-4.4124	0.2735
C	-0.6323	-3.0486	0.2723
H	-1.6282	-2.7360	0.5825
H	-1.0597	-5.1351	0.6018
H	1.1802	-5.8999	-0.1748
H	2.8507	-4.2242	-0.9500
H	2.3052	-1.8170	-0.9230
C	-0.7611	2.2344	0.0902
C	-1.3973	1.6627	1.1568
H	0.2231	2.6767	0.2045
H	-1.2722	2.4002	-0.8533
H	-0.9214	1.6524	2.1343
H	-2.4438	1.3759	1.0874

14
Gasphase Energy: -948.1389
Solvation Phase Energy: -948.1460
Zero Point Energy: 165.73 kcal/mol
Coordinates:

Ir	-0.4681	0.0799	-0.3432
O	-1.2233	0.2652	-2.2540
O	1.3370	0.0482	-1.2606
C	2.4178	-0.0889	-0.5917
C	2.5865	-0.2162	0.7876
C	1.5543	-0.2206	1.7360
O	0.3032	-0.1017	1.5423
H	1.8382	-0.3380	2.7888
H	3.6006	-0.3268	1.1551
H	3.3173	-0.1042	-1.2176
O	-0.4067	-2.1427	-0.4870
C	-0.7128	-2.6998	-1.5750

C -1.3747 -0.7502 -3.0205
C -1.1711 -2.1069 -2.7725
H -0.6155 -3.7980 -1.5950
H -1.7300 -0.4851 -4.0247
H -1.3755 -2.7803 -3.5987
C -0.5143 2.1591 -0.2261
H 0.1628 2.5001 0.5661
H -0.2078 2.5996 -1.1799
C -1.9774 2.4801 0.1315
H -2.1060 3.4110 0.6980
H -2.5847 2.5527 -0.7775
C -3.0319 -1.0548 2.4264
C -3.1109 -1.0802 1.0472
C -2.8040 0.0785 0.2841
C -2.4195 1.2767 0.9441
C -2.3608 1.2805 2.3537
C -2.6705 0.1412 3.0788
H -3.2613 -1.9428 3.0072
H -3.4203 -1.9827 0.5297
H -3.0964 0.1168 -0.7602
H -2.0671 2.1925 2.8657
H -2.6281 0.1673 4.1646

15
Gasphase Energy: -948.1192
Solvation Phase Energy: -948.1294
Zero Point Energy: 165.38 kcal/mol
Coordinates:
Ir -0.3349 0.0020 -0.4363
O -1.1617 -0.0327 -2.3070
O 1.4670 0.1709 -1.2271
C 2.5093 0.2636 -0.4779
C 2.6042 0.2666 0.9082
C 1.5202 0.1508 1.7957
O 0.2908 0.0409 1.4974
H 1.7364 0.1504 2.8697
H 3.5963 0.3554 1.3358
H 3.4294 0.3468 -1.0641
O -0.2038 -2.2152 -0.3985
C -0.4770 -2.8866 -1.4325
C -1.2741 -1.1051 -3.0029
C -0.9566 -2.4206 -2.6746
H -0.3349 -3.9755 -1.3477
H -1.6959 -0.9301 -3.9999
H -1.1322 -3.1664 -3.4427

C	-0.5587	2.0588	-0.4323
H	0.3591	2.5484	-0.0812
H	-0.7324	2.3784	-1.4666
C	-1.7440	2.4811	0.4579
H	-2.6530	1.9451	0.1466
H	-1.5424	2.1905	1.4962
C	-2.4545	6.7533	0.2230
C	-1.5580	6.2384	1.1627
C	-1.3424	4.8615	1.2448
C	-2.0157	3.9741	0.3928
C	-2.9112	4.5039	-0.5467
C	-3.1312	5.8802	-0.6321
H	-2.6264	7.8242	0.1598
H	-1.0293	6.9090	1.8352
H	-0.6459	4.4666	1.9815
H	-3.4424	3.8291	-1.2144
H	-3.8338	6.2700	-1.3641

16
Gasphase Energy: -1180.3963
Solvation Phase Energy: -1180.4044
Zero Point Energy: 230.15 kcal/mol
Coordinates:

Ir	0.4290	-0.9554	-0.0919
O	2.0753	-1.1388	1.4326
C	1.8901	-1.8411	2.4649
C	0.7097	-2.4795	2.8943
C	-0.5307	-2.4656	2.2550
O	-0.8925	-1.9151	1.1610
H	-1.3460	-3.0009	2.7590
H	0.7653	-3.0341	3.8254
H	2.7664	-1.9632	3.1228
O	1.7545	0.0102	-1.3241
C	-1.9698	1.2242	0.2898
C	-0.5675	1.2249	0.0167
H	-2.6667	1.3344	-0.5352
H	-0.2159	1.5464	-0.9564
C	-2.4279	1.1105	1.5812
C	0.3452	1.1286	1.0936
C	-1.5101	1.0148	2.6613
C	-0.1542	1.0295	2.4275
H	-1.8864	0.9468	3.6783
H	0.5498	0.9843	3.2520
H	-3.4951	1.1130	1.7837
H	1.3937	1.3534	0.9374

O	1.0290	-2.8239	-0.6229
C	1.9883	-2.9908	-1.4507
C	2.5859	-0.6427	-2.0332
C	2.7397	-2.0320	-2.1335
H	2.2300	-4.0441	-1.6325
H	3.2565	-0.0163	-2.6328
H	3.5141	-2.3961	-2.7993
C	-0.9020	-1.1198	-1.7136
H	-0.3189	-1.6034	-2.5090
H	-1.1947	-0.1395	-2.1036
C	-2.1600	-1.9600	-1.4352
H	-2.7344	-1.5096	-0.6196
H	-1.8578	-2.9529	-1.0851
C	-4.6238	-2.2936	-4.9908
C	-4.9135	-1.3299	-4.0219
C	-4.1257	-1.2332	-2.8727
C	-3.0359	-2.0917	-2.6652
C	-2.7591	-3.0556	-3.6472
C	-3.5423	-3.1581	-4.7980
H	-5.2368	-2.3738	-5.8843
H	-5.7563	-0.6564	-4.1580
H	-4.3629	-0.4858	-2.1178
H	-1.9221	-3.7355	-3.5005
H	-3.3117	-3.9159	-5.5429

17
Gasphase Energy: -1180.3945
Solvation Phase Energy: -1180.4037
Zero Point Energy: 229.31 kcal/mol
Coordinates:

Ir	-1.2494	0.4656	0.0150
H	0.4426	1.2874	0.0786
O	-1.6510	0.3465	-2.1622
O	-0.5290	-1.4438	-0.0961
C	-0.4715	0.5760	4.8211
C	-1.5605	1.2481	4.2597
C	-1.7774	1.2154	2.8791
C	-0.9129	0.5099	2.0243
C	0.1752	-0.1653	2.6058
C	0.3963	-0.1314	3.9868
H	-0.3028	0.6020	5.8945
H	-2.2451	1.8025	4.8977
H	-2.6240	1.7494	2.4583
H	0.8563	-0.7337	1.9766
H	1.2470	-0.6625	4.4082

C	1.1888	1.0741	-0.7586
H	0.9529	0.2128	-1.3806
H	2.0728	0.8253	-0.1622
C	1.3680	2.3540	-1.5889
H	1.6089	3.1919	-0.9260
H	0.4196	2.5958	-2.0791
C	-3.4838	-1.2960	0.4067
O	-3.1513	-0.0611	0.3245
H	-4.5552	-1.4370	0.5805
C	-2.4936	2.9770	-0.9152
O	-1.9361	2.4089	0.0861
H	-2.8618	3.9855	-0.6893
C	-2.2640	1.2830	-2.7491
C	-2.6838	2.5196	-2.2204
H	-2.4863	1.1130	-3.8147
H	-3.1931	3.1953	-2.8995
C	-1.3055	-2.4415	0.0499
C	-2.6852	-2.4326	0.2963
H	-0.8110	-3.4153	-0.0377
H	-3.1780	-3.3930	0.3953
C	4.4793	1.8006	-4.5491
C	4.7489	2.5091	-3.3765
C	3.7439	2.6964	-2.4241
C	2.4571	2.1827	-2.6295
C	2.1980	1.4716	-3.8112
C	3.1992	1.2816	-4.7640
H	5.2591	1.6555	-5.2913
H	5.7404	2.9184	-3.2023
H	3.9586	3.2516	-1.5136
H	1.2025	1.0670	-3.9818
H	2.9800	0.7317	-5.6753

18
Gasphase Energy: -948.1517
Solvation Phase Energy: -948.1596
Zero Point Energy: 164.74 kcal/mol
Coordinates:

Ir	-0.3262	-0.0299	-0.2493
O	-1.8267	-0.3615	-1.6189
O	0.9288	0.2501	-1.8823
C	2.1637	0.5110	-1.7152
C	2.8794	0.6607	-0.5213
C	2.3593	0.5347	0.7708
O	1.1623	0.2852	1.1301
H	3.0557	0.6659	1.6076

H	3.9377	0.8810	-0.6061
H	2.7265	0.6298	-2.6498
O	0.3998	-2.1177	-0.4216
C	-0.1423	-2.9041	-1.2476
C	-1.9561	-1.4769	-2.2294
C	-1.2337	-2.6649	-2.1048
H	0.2981	-3.9128	-1.2984
H	-2.7787	-1.4775	-2.9558
H	-1.5434	-3.4867	-2.7417
C	-1.7405	0.4953	1.4215
C	-1.5179	-0.8899	1.3381
H	-1.1008	1.0497	2.1038
H	-0.8110	-1.3554	2.0171
H	-2.2735	-1.5510	0.9239
C	-5.3225	2.6626	0.4467
C	-5.2259	1.3088	0.1127
C	-4.0705	0.5890	0.4109
C	-2.9847	1.2115	1.0475
C	-3.0964	2.5711	1.3826
C	-4.2521	3.2923	1.0856
H	-6.2247	3.2204	0.2116
H	-6.0552	0.8111	-0.3824
H	-4.0106	-0.4584	0.1376
H	-2.2631	3.0651	1.8769
H	-4.3163	4.3436	1.3522
H	-0.6094	1.5115	-0.3296

19
Gasphase Energy: -638.4365
Solvation Phase Energy: -638.4523
Zero Point Energy: 78.91 kcal/mol
Coordinates:

O	-1.7024	-0.0814	-1.8077
O	1.1609	0.2498	-1.7276
C	2.3926	0.3930	-1.3837
C	2.9605	0.4260	-0.1172
C	2.2540	0.2731	1.0886
O	1.0041	0.1104	1.2291
H	2.8255	0.2864	2.0233
H	4.0350	0.5549	-0.0583
H	3.0493	0.4948	-2.2526
O	-0.1001	-2.1683	-0.2941
C	-0.7272	-2.8937	-1.1179
C	-2.0543	-1.1818	-2.3659
C	-1.6295	-2.4861	-2.1196

H -0.5551 -3.9780 -1.0290
H -2.8163 -1.0463 -3.1426
H -2.0718 -3.2643 -2.7326
H -0.4104 1.5948 -0.3427
Ir -0.2560 0.0322 -0.3680

20
Gasphase Energy: -309.6538
Solvation Phase Energy: -309.6572
Zero Point Energy: 83.85 kcal/mol
Coordinates:
C 0.2476 -0.6826 -0.0001
C -0.4747 0.5236 0.0001
C -1.8807 0.4523 0.0003
C -2.5328 -0.7779 0.0002
C -1.7986 -1.9689 -0.0001
C -0.4040 -1.9159 -0.0002
H 1.3345 -0.6468 -0.0002
H -2.4688 1.3653 0.0005
H -3.6190 -0.8100 0.0002
H -2.3109 -2.9269 -0.0002
H 0.1777 -2.8336 -0.0004
C -0.2366 3.0361 -0.0004
C 0.2678 1.7959 0.0002
H 0.4164 3.9029 -0.0002
H 1.3520 1.6846 0.0007
H -1.3041 3.2372 -0.0010

21
Gasphase Energy: -717.0862
Solvation Phase Energy: -717.1037
Zero Point Energy: 113.58 kcal/mol
Coordinates:
O -1.5979 0.0576 -1.8935
O 1.1099 0.1524 -1.7624
C 2.3620 0.1895 -1.5322
C 3.0200 0.1475 -0.3004
C 2.3828 0.0643 0.9394
O 1.1354 0.0363 1.1992
H 3.0195 0.0280 1.8318
H 4.1039 0.1771 -0.3063
H 2.9813 0.2568 -2.4350
O -0.0195 -2.1574 -0.4138
C -0.5604 -2.7999 -1.3556

C	-1.8377	-1.0062	-2.5655
C	-1.4175	-2.3208	-2.3686
H	-0.3339	-3.8787	-1.3904
H	-2.4842	-0.8253	-3.4337
H	-1.7699	-3.0499	-3.0911
H	-0.3865	1.6130	-0.2874
Ir	-0.3175	0.0491	-0.2735
C	-1.5247	0.4367	1.5621
C	-2.2051	-0.4918	0.7604
H	-0.8901	0.0920	2.3864
H	-2.1422	-1.5715	0.9499
H	-3.0307	-0.1504	0.1192
H	-1.8399	1.4824	1.5866

22
Gasphase Energy: -717.0678
Solvation Phase Energy: -717.0778
Zero Point Energy: 114.19 kcal/mol
Coordinates:

Ir	-0.2406	0.0612	-0.3928
O	-1.5095	-0.1500	-1.9837
O	1.3087	0.1222	-1.6176
C	2.5034	0.2599	-1.1593
C	2.9382	0.3935	0.1539
C	2.1084	0.3897	1.2882
O	0.8438	0.2789	1.3138
H	2.5831	0.4889	2.2707
H	4.0052	0.4980	0.3136
H	3.2514	0.2637	-1.9575
O	-0.0696	-2.1479	-0.1653
C	-0.6203	-2.9172	-1.0005
C	-1.8080	-1.2898	-2.4928
C	-1.4223	-2.5719	-2.1090
H	-0.4646	-3.9954	-0.8353
H	-2.4796	-1.2135	-3.3563
H	-1.8062	-3.3909	-2.7080
C	-0.5365	2.1007	-0.4764
H	0.4003	2.6439	-0.2980
H	-0.8951	2.3560	-1.4800
C	-1.5791	2.4626	0.5858
H	-2.5063	1.8845	0.4608
H	-1.2023	2.2810	1.5988
H	-1.8686	3.5217	0.5276

23
Gasphase Energy: -638.4735
Solvation Phase Energy: -638.4867
Zero Point Energy: 78.66 kcal/mol
Coordinates:

Ir	0.0680	-0.6132	-0.0001
O	1.5595	-0.5127	1.3884
C	1.3153	-0.5472	2.6405
C	0.0787	-0.6755	3.2827
C	-1.1564	-0.8308	2.6441
O	-1.4051	-0.8535	1.3923
H	-2.0414	-0.9615	3.2777
H	0.0813	-0.6843	4.3670
H	2.2084	-0.4750	3.2723
O	-1.4050	-0.8535	-1.3917
C	-1.1562	-0.8304	-2.6434
C	0.0788	-0.6752	-3.2823
C	1.3157	-0.5476	-2.6410
O	1.5598	-0.5133	-1.3888
H	2.2092	-0.4760	-3.2720
H	0.0811	-0.6843	-4.3666
H	-2.0413	-0.9609	-3.2768
H	-0.1060	0.9114	0.0010

24
Gasphase Energy: -717.0814
Solvation Phase Energy: -717.0901
Zero Point Energy: 113.23 kcal/mol
Coordinates:

Ir	0.0749	-0.6629	0.0018
O	1.5252	-0.3767	1.4460
C	1.2139	-0.2978	2.6773
C	-0.0430	-0.4499	3.2773
C	-1.2471	-0.7097	2.6104
O	-1.4537	-0.8485	1.3616
H	-2.1485	-0.8149	3.2268
H	-0.0879	-0.3575	4.3569
H	2.0637	-0.0929	3.3402
O	-1.4017	-0.7219	-1.4431
C	-1.1154	-0.5811	-2.6749
C	0.1437	-0.4470	-3.2747
C	1.3748	-0.4222	-2.6070
O	1.6066	-0.5026	-1.3576
H	2.2769	-0.3237	-3.2235

H 0.1673 -0.3528 -4.3548
H -1.9889 -0.5784 -3.3386
H -0.1041 0.8912 -0.0025
C -0.0783 -3.1367 -0.5106
C 0.7872 -3.0346 0.5259
H -1.1388 -3.2993 -0.3505
H 0.4516 -3.1275 1.5539
H 1.8572 -2.9539 0.3659
H 0.2704 -3.1569 -1.5383

25
Gasphase Energy: -1026.7664
Solvation Phase Energy: -1026.7741
Zero Point Energy: 200.48 kcal/mol
Coordinates:
Ir -0.3207 0.0426 -0.3487
O -0.7691 0.0813 -2.3695
O 1.5942 -0.0786 -1.1230
C 2.6463 -0.2183 -0.4218
C 2.7559 -0.2528 0.9705
C 1.6759 -0.1366 1.8480
O 0.4364 0.0017 1.5850
H 1.8947 -0.1633 2.9223
H 3.7441 -0.3708 1.3996
H 3.5678 -0.3125 -1.0090
O -0.3127 -2.1951 -0.3153
C -0.4841 -2.8346 -1.3869
C -0.8234 -0.9936 -3.0656
C -0.7227 -2.3290 -2.6849
H -0.4430 -3.9329 -1.3029
H -0.9898 -0.7999 -4.1325
H -0.8260 -3.0613 -3.4788
C -0.2845 2.1318 -0.3341
H -1.3159 2.5098 -0.2960
H 0.1977 2.4448 0.6018
C 0.4272 2.7856 -1.5336
H 1.4771 2.4754 -1.5528
H -0.0228 2.4206 -2.4617
C 0.1454 7.1093 -1.3353
C -0.8035 6.3733 -2.0491
C -0.7023 4.9824 -2.1209
C 0.3441 4.2983 -1.4847
C 1.2891 5.0514 -0.7720
C 1.1939 6.4421 -0.6965
H 0.0712 8.1920 -1.2809

H -1.6201 6.8826 -2.5546
H -1.4411 4.4151 -2.6835
H 2.1107 4.5385 -0.2759
H 1.9404 7.0059 -0.1428
C -2.0981 0.1444 0.9595
C -2.5313 -0.0028 -0.3511
H -2.0260 -0.7151 1.6171
H -2.8185 -0.9779 -0.7323
H -2.8627 0.8532 -0.9298
H -2.0892 1.1166 1.4408

26
Gasphase Energy: -1026.7656
Solvation Phase Energy: -1026.7736
Zero Point Energy: 201.32 kcal/mol
Coordinates:
Ir -0.4653 0.1845 -0.4368
O -0.9727 0.1604 -2.4322
O 1.4012 -0.2096 -1.0478
C 2.3548 -0.3592 -0.2064
C 2.3236 -0.2745 1.1854
C 1.1875 -0.0026 1.9593
O 0.0019 0.2243 1.5558
H 1.3093 0.0251 3.0481
H 3.2568 -0.4404 1.7116
H 3.3148 -0.5843 -0.6831
O -0.7350 -2.0232 -0.2578
C -1.0035 -2.7012 -1.2862
C -1.1910 -0.9340 -3.0631
C -1.2179 -2.2501 -2.6070
H -1.0860 -3.7899 -1.1339
H -1.3951 -0.7812 -4.1304
H -1.4351 -3.0106 -3.3500
C -0.1867 2.2312 -0.6013
H 0.8578 2.4872 -0.3812
H -0.3782 2.4926 -1.6505
C -1.1320 3.0040 0.3275
H -0.8222 2.8618 1.3713
H -1.0715 4.0837 0.1266
C -2.5897 2.5494 0.1815
H -3.2465 3.1276 0.8439
H -2.9407 2.7256 -0.8432
C -2.7735 1.0642 0.5310
H -2.2800 0.3882 -0.2667
H -2.3476 0.8380 1.5095

C -6.8801 -0.2717 0.3288
C -6.2307 -0.1789 1.5613
C -4.8975 0.2335 1.6213
C -4.2028 0.5674 0.4520
C -4.8612 0.4664 -0.7824
C -6.1904 0.0488 -0.8444
H -7.9152 -0.5978 0.2809
H -6.7579 -0.4330 2.4768
H -4.3909 0.2977 2.5812
H -4.3236 0.7071 -1.6967
H -6.6870 -0.0304 -1.8074

27
Gasphase Energy: -1026.7355
Solvation Phase Energy: -1026.7444
Zero Point Energy: 198.96 kcal/mol
Coordinates:
Ir -1.2592 0.4721 0.0108
H 0.4396 1.2959 0.0444
O -1.7100 0.3753 -2.1613
O -0.5285 -1.4326 -0.1290
H 0.1672 -0.0189 3.7454
C 0.0329 -0.1495 2.6721
C -0.8843 0.5498 1.9939
H -1.5099 1.2672 2.5322
H 0.6831 -0.8766 2.1897
C 1.1769 1.0793 -0.7981
H 0.9149 0.2394 -1.4385
H 2.0560 0.7929 -0.2116
C 1.3853 2.3722 -1.6013
H 1.6363 3.1926 -0.9203
H 0.4448 2.6410 -2.0934
C -3.4768 -1.3118 0.4132
O -3.1524 -0.0729 0.3583
H -4.5448 -1.4626 0.6001
C -2.5115 2.9981 -0.8550
O -1.9541 2.4085 0.1337
H -2.8747 4.0039 -0.6092
C -2.3116 1.3336 -2.7233
C -2.7095 2.5663 -2.1678
H -2.5460 1.1896 -3.7904
H -3.2155 3.2598 -2.8313
C -1.2977 -2.4369 0.0039
C -2.6754 -2.4416 0.2623
H -0.7982 -3.4062 -0.1045

H	-3.1624	-3.4066	0.3441
C	4.5155	1.8219	-4.5428
C	4.7886	2.4911	-3.3481
C	3.7772	2.6778	-2.4025
C	2.4802	2.2026	-2.6360
C	2.2177	1.5315	-3.8399
C	3.2253	1.3422	-4.7863
H	5.3004	1.6770	-5.2798
H	5.7879	2.8700	-3.1514
H	3.9951	3.2021	-1.4746
H	1.2145	1.1576	-4.0337
H	3.0033	0.8235	-5.7150

TS1A
Gasphase Energy: -869.4902
Solvation Phase Energy: -869.4998
Zero Point Energy: 129.91 kcal/mol
Imaginary Frequency: -84.30 cm-1
Coordinates:

Ir	-0.1066	0.0289	0.0141
O	-0.1877	-0.0140	2.0626
O	1.8633	-0.2301	0.1091
C	2.5697	-0.3285	-0.9601
C	2.1683	-0.2763	-2.2899
C	0.8536	-0.0587	-2.7317
O	-0.1866	0.1067	-2.0205
H	0.6807	-0.0033	-3.8120
H	2.9383	-0.3849	-3.0449
H	3.6340	-0.4567	-0.7419
C	-0.2134	-1.9915	-0.0280
C	-1.1122	-2.6116	-0.9125
C	-1.2949	-3.9987	-0.8933
C	-0.5718	-4.7914	-0.0001
C	0.3345	-4.1858	0.8746
C	0.5155	-2.8001	0.8585
H	1.2163	-2.3417	1.5500
H	0.9017	-4.7931	1.5761
H	-0.7105	-5.8691	0.0127
H	-1.9998	-4.4564	-1.5834
H	-1.6736	-2.0116	-1.6248
O	-0.7801	2.1021	0.0151
C	-0.9812	2.7469	1.0941
C	-0.4535	1.0006	2.7913
C	-0.8115	2.2981	2.4107
H	-1.3372	3.7796	0.9664

H	-0.4045	0.7913	3.8664
H	-1.0149	3.0046	3.2081

TS1B
Gasphase Energy: -948.0873
Solvation Phase Energy: -948.0960
Zero Point Energy: 162.65 kcal/mol
Imaginary Frequency: -132.47 cm-1
Coordinates:

Ir	-0.0216	0.0004	-0.0116
O	-0.0937	0.0035	2.0282
C	0.9702	0.0373	2.7267
C	2.2974	0.0927	2.2791
C	2.6977	0.1458	0.9457
O	1.9775	0.1242	-0.1143
H	3.7665	0.2352	0.7287
H	3.0766	0.1240	3.0321
H	0.7996	0.0381	3.8092
O	-0.0287	0.0576	-2.0646
C	-0.7469	0.8496	-2.7553
C	-1.6729	1.8096	-2.3241
C	-1.9864	2.1030	-0.9925
O	-1.5184	1.5707	0.0668
H	-2.7343	2.8922	-0.8268
H	-2.1809	2.3814	-3.0931
H	-0.6023	0.7470	-3.8377
C	0.3780	-1.9887	-0.0340
C	1.1465	-2.5591	-1.0606
C	1.3564	-3.9409	-1.1101
C	0.8131	-4.7764	-0.1313
C	0.0582	-4.2158	0.9010
C	-0.1550	-2.8339	0.9531
H	-0.7371	-2.4154	1.7683
H	-0.3669	-4.8513	1.6742
H	0.9779	-5.8497	-0.1712
H	1.9473	-4.3629	-1.9197
H	1.5730	-1.9225	-1.8289
C	-2.9986	-1.5046	-1.0024
C	-3.3194	-1.1421	0.2416
H	-3.3405	-0.9398	-1.8655
H	-3.9299	-0.2679	0.4476
H	-2.9797	-1.7094	1.1025
H	-2.3773	-2.3727	-1.1977

TS2
Gasphase Energy: -948.1027
Solvation Phase Energy: -948.1100
Zero Point Energy: 164.56 kcal/mol
Imaginary Frequency: -349.24 cm-1
Coordinates:

Ir	-0.0178	0.0607	0.0113
O	-0.0769	0.0341	2.0695
O	2.1444	-0.2063	0.1273
C	2.8384	-0.1812	-0.9262
C	2.4117	0.0002	-2.2584
C	1.1005	0.1530	-2.7022
O	0.0016	0.1494	-2.0436
H	0.9573	0.2804	-3.7826
H	3.1844	0.0149	-3.0198
H	3.9216	-0.3166	-0.7816
C	-0.3418	-2.1171	-0.0238
C	0.0654	-2.8130	1.1355
C	0.6210	-4.0880	1.0507
C	0.7694	-4.7107	-0.1923
C	0.3531	-4.0472	-1.3525
C	-0.2028	-2.7743	-1.2678
H	-0.5419	-2.2713	-2.1678
H	0.4571	-4.5268	-2.3221
H	1.1970	-5.7073	-0.2569
H	0.9410	-4.5960	1.9565
H	-0.0400	-2.3303	2.1011
O	0.4839	2.0707	-0.0869
C	0.6287	2.7643	0.9682
C	0.1753	1.0825	2.7529
C	0.5003	2.3652	2.3064
H	0.8869	3.8151	0.7841
H	0.1180	0.9300	3.8374
H	0.6716	3.1210	3.0650
C	-2.0210	-1.2514	0.1535
C	-2.0827	0.2008	-0.0340
H	-2.4824	-1.8653	-0.6136
H	-2.4469	0.5466	-1.0011
H	-2.4771	0.7723	0.8068
H	-2.2358	-1.6024	1.1585

TS2 optimized in solvent
Solvation Phase Energy: -948.1106
Zero Point Energy: 164.49 kcal/mol
Imaginary Frequency: -349.90 cm-1

Coordinates:

Ir	-0.0112	0.0630	0.0144
O	-0.0672	0.0377	2.0742
O	2.1545	-0.2084	0.1140
C	2.8426	-0.2073	-0.9459
C	2.4070	-0.0385	-2.2765
C	1.0957	0.1316	-2.7130
O	0.0021	0.1540	-2.0430
H	0.9461	0.2521	-3.7931
H	3.1740	-0.0450	-3.0441
H	3.9248	-0.3526	-0.8071
C	-0.3361	-2.1147	-0.0281
C	0.0687	-2.8154	1.1299
C	0.6170	-4.0942	1.0433
C	0.7597	-4.7171	-0.2013
C	0.3443	-4.0496	-1.3602
C	-0.2037	-2.7728	-1.2727
H	-0.5460	-2.2711	-2.1721
H	0.4409	-4.5297	-2.3307
H	1.1805	-5.7169	-0.2676
H	0.9339	-4.6062	1.9485
H	-0.0353	-2.3360	2.0975
O	0.4802	2.0791	-0.0778
C	0.5978	2.7812	0.9779
C	0.1532	1.0937	2.7604
C	0.4574	2.3821	2.3144
H	0.8404	3.8355	0.7939
H	0.0863	0.9410	3.8440
H	0.6027	3.1431	3.0738
C	-2.0224	-1.2502	0.1470
C	-2.0771	0.2048	-0.0129
H	-2.4759	-1.8464	-0.6379
H	-2.4507	0.5691	-0.9698
H	-2.4614	0.7634	0.8415
H	-2.2464	-1.6243	1.1415

TS2(2,2)-propene
Gasphase Energy: -987.4201
Solvation Phase Energy: -987.4281
Zero Point Energy: 182.22 kcal/mol
Imaginary Frequency: -333.37 cm-1
Coordinates:

Ir	-0.0156	0.0614	0.0247
O	-0.0106	0.0535	2.0862
O	2.1505	-0.2119	0.0868

C	2.8168	-0.2051	-0.9845
C	2.3547	-0.0413	-2.3072
C	1.0329	0.1160	-2.7175
O	-0.0483	0.1310	-2.0303
H	0.8627	0.2299	-3.7955
H	3.1065	-0.0427	-3.0896
H	3.9032	-0.3428	-0.8672
C	-0.3638	-2.1131	0.0029
C	0.1376	-2.7679	1.1509
C	0.7698	-4.0069	1.0594
C	0.8969	-4.6428	-0.1789
C	0.3831	-4.0288	-1.3273
C	-0.2433	-2.7896	-1.2337
H	-0.6451	-2.3228	-2.1279
H	0.4713	-4.5186	-2.2934
H	1.3859	-5.6107	-0.2489
H	1.1704	-4.4733	1.9555
H	0.0643	-2.2759	2.1136
O	0.4808	2.0720	-0.0993
C	0.6794	2.7697	0.9434
C	0.2819	1.1024	2.7538
C	0.6044	2.3784	2.2884
H	0.9411	3.8166	0.7423
H	0.2669	0.9558	3.8407
H	0.8177	3.1352	3.0352
C	-2.1051	-1.2721	0.1382
C	-2.0773	0.1951	0.0329
H	-2.4511	-1.7683	-0.7645
H	-2.4471	0.6031	-0.9084
H	-2.4586	0.7284	0.9065
C	-2.6832	-1.8588	1.4113
H	-2.2095	-1.4160	2.2906
H	-3.7497	-1.6018	1.4408
H	-2.5800	-2.9450	1.4576

TS2(1,2)-propene
Gasphase Energy: -987.4197
Solvation Phase Energy: -987.4265
Zero Point Energy: 182.10 kcal/mol
Imaginary Frequency: -335.45 cm-1
Coordinates:

Ir	-0.0230	0.0581	-0.0015
O	-0.1245	0.0516	2.0545
O	2.1488	-0.2138	0.1678
C	2.8765	-0.1973	-0.8617

C	2.4894	-0.0277	-2.2077
C	1.1911	0.1189	-2.6878
O	0.0732	0.1220	-2.0615
H	1.0782	0.2351	-3.7732
H	3.2829	-0.0192	-2.9475
H	3.9553	-0.3307	-0.6832
C	-0.3463	-2.1218	-0.0324
C	0.0624	-2.8057	1.1340
C	0.6385	-4.0718	1.0607
C	0.8062	-4.6991	-0.1779
C	0.3891	-4.0480	-1.3445
C	-0.1868	-2.7831	-1.2714
H	-0.5234	-2.2892	-2.1772
H	0.5082	-4.5306	-2.3109
H	1.2494	-5.6895	-0.2337
H	0.9584	-4.5698	1.9720
H	-0.0603	-2.3201	2.0962
O	0.4898	2.0631	-0.1073
C	0.6281	2.7647	0.9434
C	0.1305	1.1024	2.7339
C	0.4768	2.3779	2.2827
H	0.9000	3.8109	0.7537
H	0.0554	0.9587	3.8185
H	0.6463	3.1375	3.0378
C	-2.0089	-1.2594	0.1242
C	-2.0966	0.2041	-0.0239
H	-2.4726	-1.8398	-0.6691
H	-2.4166	0.7071	0.8929
H	-2.2433	-1.6408	1.1137
C	-2.7619	0.7714	-1.2657
H	-2.5306	1.8359	-1.3728
H	-2.4132	0.2694	-2.1717
H	-3.8550	0.6702	-1.2107

TS2(2,2,2)-butene
Gasphase Energy: -1184.0345
Solvation Phase Energy: -1184.0393
Zero Point Energy: 268.83 kcal/mol
Imaginary Frequency: -326.85 cm-1
Coordinates: Ir -0.0132 0.0438 0.0209

O	-0.0089	0.0454	2.0792
O	2.1459	-0.2051	0.0730
C	2.8458	-0.1491	-0.9809
C	2.3735	0.0415	-2.3037
C	1.0496	0.1628	-2.7381

O	-0.0258	0.1138	-2.0329
H	3.1308	0.0903	-3.0773
C	-0.3705	-2.1377	0.0117
C	0.0387	-2.7788	1.2052
C	0.7336	-3.9863	1.1875
C	1.0305	-4.6090	-0.0288
C	0.6305	-4.0061	-1.2257
C	-0.0637	-2.7986	-1.2014
H	-0.3505	-2.3400	-2.1398
H	0.8655	-4.4741	-2.1782
H	1.5706	-5.5520	-0.0444
H	1.0542	-4.4366	2.1234
H	-0.1481	-2.2926	2.1546
O	0.4539	2.0536	-0.0889
C	0.6615	2.7750	0.9426
C	0.2936	1.0818	2.7700
C	0.6004	2.3626	2.2875
H	0.8216	3.1167	3.0331
C	-2.1673	-1.3113	0.0546
C	-2.0694	0.1662	0.0226
C	0.7791	0.3546	-4.2166
H	0.2359	1.2934	-4.3672
H	1.6959	0.3722	-4.8088
H	0.1334	-0.4521	-4.5808
C	4.3406	-0.3080	-0.7682
H	4.9131	-0.2124	-1.6933
H	4.6849	0.4437	-0.0506
H	4.5380	-1.2901	-0.3254
C	1.0041	4.2156	0.6265
H	1.1793	4.8092	1.5257
H	1.8981	4.2446	-0.0048
H	0.1881	4.6655	0.0513
C	0.3163	0.8313	4.2627
H	0.4665	1.7479	4.8361
H	-0.6218	0.3599	4.5722
H	1.1248	0.1300	4.4975
H	-2.4378	0.6268	-0.8964
H	-2.4529	0.6648	0.9165
C	-2.8073	-1.9146	-1.1878
H	-2.3727	-1.4984	-2.0987
H	-2.7358	-3.0047	-1.2129
H	-3.8683	-1.6325	-1.1705
C	-2.7246	-1.8734	1.3544
H	-2.6530	-2.9626	1.4055
H	-2.2239	-1.4356	2.2198
H	-3.7841	-1.5893	1.4025

TS2(1,1,2)-butene
Gasphase Energy: -1184.0349
Solvation Phase Energy: -1184.0376
Zero Point Energy: 268.58 kcal/mol
Imaginary Frequency: -316.08 cm-1
Coordinates: Ir -0.0734 0.0689 0.0024

O	-0.0742	0.0599	2.0596
O	2.0981	-0.1782	0.1583
C	2.8512	-0.1534	-0.8587
C	2.4480	0.0328	-2.2041
C	1.1481	0.1647	-2.7010
O	0.0370	0.1294	-2.0528
H	3.2414	0.0621	-2.9415
C	-0.3432	-2.1283	-0.0329
C	0.0617	-2.7966	1.1436
C	0.6931	-4.0370	1.0866
C	0.9243	-4.6555	-0.1464
C	0.5130	-4.0196	-1.3237
C	-0.1191	-2.7810	-1.2666
H	-0.4519	-2.3007	-2.1810
H	0.6801	-4.4943	-2.2871
H	1.4104	-5.6262	-0.1899
H	1.0069	-4.5220	2.0073
H	-0.1071	-2.3162	2.1013
O	0.4376	2.0627	-0.0972
C	0.7060	2.7628	0.9371
C	0.3087	1.0669	2.7537
C	0.6680	2.3366	2.2769
H	0.9474	3.0695	3.0240
C	-1.9996	-1.3085	0.0807
C	-2.1629	0.1624	-0.0588
H	-2.4324	-1.8943	-0.7267
H	-2.2707	-1.6989	1.0585
C	0.9503	0.3551	-4.1911
H	0.4339	1.3044	-4.3686
H	1.8934	0.3518	-4.7407
H	0.3047	-0.4392	-4.5810
C	4.3282	-0.3515	-0.5708
H	4.9525	-0.2394	-1.4598
H	4.6477	0.3662	0.1914
H	4.4787	-1.3533	-0.1540
C	1.1010	4.1901	0.6250
H	1.2990	4.7735	1.5261
H	1.9958	4.1874	-0.0062

H	0.3030	4.6720	0.0510
C	0.3398	0.8009	4.2429
H	0.6394	1.6801	4.8160
H	-0.6500	0.4735	4.5783
H	1.0389	-0.0164	4.4495
C	-2.7570	0.6404	-1.3812
H	-2.5758	1.7123	-1.5155
H	-2.3200	0.1261	-2.2383
H	-3.8460	0.4837	-1.3928
C	-2.8203	0.8657	1.1273
H	-2.6013	1.9391	1.1114
H	-3.9141	0.7557	1.0848
H	-2.4758	0.4636	2.0822

TS2(2,2)-styrene
Gasphase Energy: -1179.1538
Solvation Phase Energy: -1179.1620
Zero Point Energy: 215.16 kcal/mol
Imaginary Frequency: -322.52 cm-1
Coordinates:

Ir	0.0598	0.1302	0.0295
O	0.3177	0.3067	2.0686
O	2.2251	-0.0928	-0.1396
C	2.7648	-0.1555	-1.2778
C	2.1491	-0.1096	-2.5468
C	0.7844	-0.0204	-2.8114
O	-0.2117	0.0209	-2.0060
H	0.4891	0.0005	-3.8681
H	2.8066	-0.1551	-3.4089
H	3.8616	-0.2582	-1.2775
C	-0.2441	-2.0466	0.2277
C	0.3277	-2.5775	1.4064
C	1.0080	-3.7919	1.3945
C	1.1017	-4.5338	0.2116
C	0.5112	-4.0491	-0.9610
C	-0.1573	-2.8274	-0.9486
H	-0.6105	-2.4548	-1.8621
H	0.5754	-4.6226	-1.8820
H	1.6238	-5.4870	0.2055
H	1.4646	-4.1630	2.3080
H	0.2549	-2.0124	2.3276
O	0.4595	2.1369	-0.3176
C	0.7888	2.9230	0.6238
C	0.6803	1.4098	2.6005
C	0.9128	2.6450	1.9931

H	0.9967	3.9517	0.3015
H	0.8167	1.3544	3.6877
H	1.2155	3.4624	2.6385
C	-2.0405	-1.2602	0.3740
C	-1.9947	0.2083	0.2723
H	-2.3647	-1.7382	-0.5459
H	-2.4643	0.5986	-0.6320
H	-2.3035	0.7559	1.1630
C	-3.6796	-3.2967	3.7959
C	-3.0675	-2.0512	3.9609
C	-2.5283	-1.3789	2.8642
C	-2.5863	-1.9492	1.5830
C	-3.1969	-3.2045	1.4290
C	-3.7449	-3.8716	2.5238
H	-4.0993	-3.8169	4.6523
H	-3.0088	-1.6013	4.9482
H	-2.0346	-0.4237	3.0036
H	-3.2306	-3.6628	0.4433
H	-4.2167	-4.8404	2.3852

TS2(1,2)-styrene
Gasphase Energy: -1179.1561
Solvation Phase Energy: -1179.1640
Zero Point Energy: 215.39 kcal/mol
Imaginary Frequency: -328.24 cm-1
Coordinates:

Ir	0.0322	0.0371	-0.0324
O	-0.1423	0.1197	2.0195
O	2.1701	-0.2599	0.2452
C	2.9468	-0.2972	-0.7507
C	2.6273	-0.1783	-2.1169
C	1.3519	-0.0314	-2.6601
O	0.2118	0.0143	-2.0821
H	1.2856	0.0424	-3.7528
H	3.4536	-0.2130	-2.8190
H	4.0119	-0.4391	-0.5114
C	-0.3357	-2.1291	0.0086
C	0.0436	-2.7907	1.1978
C	0.5691	-4.0805	1.1674
C	0.7163	-4.7527	-0.0502
C	0.3331	-4.1212	-1.2395
C	-0.1913	-2.8324	-1.2097
H	-0.4915	-2.3517	-2.1349
H	0.4404	-4.6370	-2.1900
H	1.1193	-5.7614	-0.0728

H	0.8660	-4.5616	2.0955
H	-0.0648	-2.2707	2.1437
O	0.5933	2.0281	-0.2028
C	0.7161	2.7671	0.8228
C	0.1200	1.1919	2.6630
C	0.5127	2.4382	2.1717
H	1.0196	3.7984	0.6012
H	0.0074	1.0956	3.7496
H	0.6782	3.2238	2.9008
C	-1.9785	-1.2259	0.1579
C	-2.0635	0.2167	-0.1222
H	-2.4878	-1.8845	-0.5383
H	-2.3577	0.8047	0.7493
H	-2.1750	-1.4849	1.1932
C	-3.9291	1.8153	-3.6719
C	-3.7777	2.5927	-2.5212
C	-3.1710	2.0544	-1.3869
C	-2.6948	0.7318	-1.3704
C	-2.8537	-0.0359	-2.5367
C	-3.4642	0.4979	-3.6714
H	-4.4040	2.2294	-4.5570
H	-4.1364	3.6185	-2.5047
H	-3.0612	2.6649	-0.4934
H	-2.4923	-1.0592	-2.5680
H	-3.5762	-0.1187	-4.5596

TS2(2,2)-VTFM
Gasphase Energy: -1285.1302
Solvation Phase Energy: -1285.1376
Zero Point Energy: 167.67 kcal/mol
Imaginary Frequency: -314.57 cm-1
Coordinates:

Ir	0.4684	0.4093	0.0795
O	0.6339	0.4136	2.1330
O	2.6263	0.2245	-0.0278
C	3.2097	0.2799	-1.1460
C	2.6458	0.4502	-2.4278
C	1.2917	0.5404	-2.7368
O	0.2684	0.4784	-1.9665
H	3.3377	0.5017	-3.2618
C	0.2534	-1.7589	0.1097
C	0.6014	-2.3846	1.3276
C	1.1620	-3.6597	1.3394
C	1.3686	-4.3540	0.1440
C	1.0083	-3.7614	-1.0710

C	0.4489	-2.4875	-1.0859
H	0.1621	-2.0402	-2.0320
H	1.1598	-4.2942	-2.0057
H	1.7996	-5.3512	0.1584
H	1.4396	-4.1127	2.2872
H	0.4525	-1.8530	2.2579
O	0.8931	2.4405	-0.0726
C	1.1283	3.1528	0.9537
C	0.9177	1.4752	2.7809
C	1.1509	2.7660	2.2996
H	1.3766	3.5326	3.0324
C	-1.5129	-0.8919	-0.0040
C	-1.5961	0.5422	0.2526
H	-2.0114	1.1411	-0.5556
H	-1.9278	0.8413	1.2458
H	-1.6895	-1.1633	-1.0402
C	-2.3362	-1.7911	0.9087
F	-2.2004	-3.1037	0.6545
F	-2.0862	-1.5855	2.2157
F	-3.6402	-1.4873	0.6956
H	1.0311	0.6605	-3.7954
H	4.3054	0.1841	-1.1091
H	1.3377	4.2073	0.7320
H	0.9791	1.3271	3.8657

TS2(1,2)-VTFM
Gasphase Energy: -1285.1399
Solvation Phase Energy: -1285.1476
Zero Point Energy: 167.86 kcal/mol
Imaginary Frequency: -328.02 cm-1
Coordinates:

Ir	-0.0027	0.0841	-0.0056
O	-0.1442	0.0866	2.0512
O	2.1161	-0.1874	0.2452
C	2.8943	-0.1962	-0.7530
C	2.5731	-0.0455	-2.1129
C	1.2935	0.1158	-2.6433
O	0.1593	0.1425	-2.0546
H	1.2171	0.2227	-3.7322
H	3.3961	-0.0601	-2.8191
H	3.9582	-0.3373	-0.5129
C	-0.2856	-2.0829	-0.0474
C	0.1719	-2.7844	1.0882
C	0.6925	-4.0719	0.9698
C	0.7526	-4.6952	-0.2804

C	0.2821	-4.0221	-1.4142
C	-0.2393	-2.7368	-1.2988
H	-0.6273	-2.2243	-2.1730
H	0.3152	-4.5045	-2.3873
H	1.1537	-5.7009	-0.3702
H	1.0550	-4.5881	1.8546
H	0.1343	-2.2997	2.0581
O	0.5226	2.0905	-0.1137
C	0.6341	2.7964	0.9354
C	0.1030	1.1434	2.7273
C	0.4543	2.4152	2.2746
H	0.9078	3.8423	0.7473
H	0.0117	1.0053	3.8111
H	0.6071	3.1795	3.0284
C	-1.9821	-1.2095	0.2171
C	-2.0787	0.2319	-0.0257
H	-2.4753	-1.8585	-0.4972
H	-2.4156	0.8276	0.8234
H	-2.1205	-1.5137	1.2487
C	-2.8017	0.6675	-1.2690
F	-2.4696	1.9177	-1.6446
F	-2.5853	-0.1558	-2.3216
F	-4.1504	0.6726	-1.0632

TS2(2,2)-VME
Gasphase Energy: -1062.6271
Solvation Phase Energy: -1062.6359
Zero Point Energy: 184.73 kcal/mol
Imaginary Frequency: -352.39 cm-1
Coordinates:

Ir	0.4673	0.3743	0.0651
O	0.8545	0.3881	2.0895
O	2.6261	0.2622	-0.2537
C	3.0930	0.3197	-1.4226
C	2.3949	0.4405	-2.6453
C	1.0146	0.4888	-2.8208
O	0.0709	0.4133	-1.9552
H	2.9986	0.5017	-3.5451
C	0.1692	-1.7956	0.1575
C	0.4316	-2.3805	1.4195
C	1.0999	-3.5975	1.5313
C	1.4993	-4.2861	0.3789
C	1.2044	-3.7609	-0.8833
C	0.5365	-2.5412	-0.9873
H	0.3136	-2.1383	-1.9708

H	1.4990	-4.2989	-1.7804
H	2.0251	-5.2333	0.4658
H	1.3184	-4.0086	2.5133
H	0.1322	-1.8480	2.3152
O	0.7600	2.4292	-0.1141
C	1.1087	3.1455	0.8752
C	1.1915	1.4554	2.7013
C	1.3265	2.7536	2.2029
H	1.6283	3.5233	2.9049
C	-1.6706	-1.0777	0.0189
C	-1.5729	0.3323	0.4085
H	-2.0945	0.9961	-0.2854
H	-1.8585	0.5095	1.4479
H	-1.7621	-1.2697	-1.0517
O	-2.4161	-1.8872	0.8087
H	0.6525	0.5846	-3.8523
H	4.1910	0.2697	-1.4990
H	1.2506	4.2083	0.6380
H	1.3983	1.3081	3.7689
C	-2.5849	-3.2344	0.3683
H	-3.3805	-3.6597	0.9815
H	-2.8749	-3.2680	-0.6889
H	-1.6608	-3.8031	0.5139

TS2(1,2)-VME
Gasphase Energy: -1062.6218
Solvation Phase Energy: -1062.6298
Zero Point Energy: 184.87 kcal/mol
Imaginary Frequency: -341.55 cm-1
Coordinates:

Ir	-0.0171	0.0836	0.0135
O	-0.1163	0.0711	2.0733
O	2.1605	-0.1931	0.1953
C	2.8890	-0.1961	-0.8340
C	2.5057	-0.0296	-2.1811
C	1.2103	0.1397	-2.6635
O	0.0910	0.1654	-2.0419
H	1.1018	0.2567	-3.7494
H	3.2995	-0.0410	-2.9206
H	3.9657	-0.3455	-0.6545
C	-0.3322	-2.0774	-0.0454
C	0.1290	-2.7998	1.0766
C	0.6441	-4.0871	0.9370
C	0.6951	-4.6936	-0.3218
C	0.2213	-4.0013	-1.4429

C	-0.2934	-2.7158	-1.3062
H	-0.6799	-2.1883	-2.1723
H	0.2481	-4.4693	-2.4234
H	1.0916	-5.6995	-0.4283
H	1.0098	-4.6169	1.8127
H	0.0975	-2.3300	2.0539
O	0.5101	2.0968	-0.0834
C	0.6617	2.7867	0.9728
C	0.1595	1.1146	2.7564
C	0.5171	2.3885	2.3103
H	0.9403	3.8334	0.7934
H	0.0904	0.9658	3.8406
H	0.7008	3.1403	3.0700
C	-1.9921	-1.1964	0.2509
C	-2.0885	0.2302	-0.0494
H	-2.5312	-1.8432	-0.4337
H	-2.4551	0.8730	0.7619
H	-2.1191	-1.4536	1.2971
O	-2.7035	0.4913	-1.2703
C	-2.6293	1.8508	-1.6680
H	-3.1818	1.9348	-2.6067
H	-3.0975	2.5099	-0.9199
H	-1.5910	2.1628	-1.8217

TS3
Gasphase Energy: -1180.3436
Solvation Phase Energy: -1180.3817
Zero Point Energy: 227.99 kcal/mol
Imaginary Frequency: -391.28 cm-1
Coordinates:

Ir	0.0022	0.0555	0.0811
O	-0.1419	0.5413	2.1398
C	0.8930	0.5681	2.8748
C	2.2283	0.3272	2.5208
C	2.6951	-0.0050	1.2478
O	2.0433	-0.1826	0.1637
H	3.7764	-0.1420	1.1311
H	2.9705	0.4147	3.3070
H	0.4918	1.3119	-2.1024
O	-2.0364	0.3483	-0.0123
O	0.3958	2.2046	0.0017
C	-0.5647	3.0304	-0.0011
C	-2.5554	1.5154	-0.0191
C	-1.9455	2.7716	-0.0124

H	-0.2665	4.0893	-0.0042
H	-3.6517	1.4976	-0.0383
H	-2.6063	3.6320	-0.0210
C	-0.2743	-1.9146	0.7051
H	-0.7945	0.1796	-2.5747
C	1.2467	-0.5793	-2.8464
H	0.9188	-1.6249	-2.9146
H	2.1720	-0.5715	-2.2623
C	-1.4312	-2.2463	1.4237
C	-1.5936	-3.5308	1.9528
C	-0.6114	-4.5057	1.7620
C	0.5364	-4.1866	1.0330
C	0.7014	-2.9019	0.5050
H	-2.2040	-1.5005	1.5756
H	-2.4941	-3.7671	2.5155
H	-0.7412	-5.5039	2.1725
H	1.3073	-4.9365	0.8703
H	1.5988	-2.6683	-0.0608
H	0.6974	0.8222	3.9250
H	-0.2038	-1.0071	-1.0690
C	0.1930	0.2621	-2.1111
C	1.9316	1.0397	-6.8080
C	0.9801	0.0349	-6.6151
C	0.7682	-0.4938	-5.3399
C	1.5018	-0.0317	-4.2379
C	2.4544	0.9771	-4.4450
C	2.6690	1.5095	-5.7177
H	2.0999	1.4506	-7.8002
H	0.4048	-0.3405	-7.4579
H	0.0288	-1.2796	-5.1967
H	3.0346	1.3428	-3.5999
H	3.4153	2.2875	-5.8589

TS4
Gasphase Energy: -948.1299
Solvation Phase Energy: -948.1387
Zero Point Energy: 163.66 kcal/mol
Imaginary Frequency: -176.62 cm-1
Coordinates:

Ir	-0.0222	-0.0312	-0.0032
O	-0.0369	-0.0108	2.0545
O	2.0374	0.0623	0.1646
C	2.7701	0.1001	-0.8748
C	2.3877	0.0855	-2.2226
C	1.0786	0.0094	-2.7068

O	-0.0145	-0.0670	-2.0529
H	0.9455	0.0061	-3.7951
H	3.1816	0.1349	-2.9596
H	3.8458	0.1487	-0.6629
O	0.2522	2.1367	-0.1253
C	0.3314	2.8220	0.9312
C	0.1144	1.0752	2.7170
C	0.2778	2.3844	2.2704
H	0.4588	3.9055	0.7821
H	0.1040	0.9238	3.8035
H	0.3781	3.1462	3.0364
C	-0.5619	-2.0310	0.0291
H	-0.2012	-2.6074	-0.8220
H	-0.4007	-2.5266	0.9849
C	-1.8704	-1.3665	-0.1618
H	-1.7182	-0.0191	-0.0825
H	-2.2121	-1.3742	-1.1978
C	-5.1921	-1.8355	2.5499
C	-5.4027	-1.7321	1.1740
C	-4.3160	-1.5663	0.3133
C	-3.0076	-1.5115	0.8139
C	-2.8033	-1.6122	2.1982
C	-3.8906	-1.7720	3.0569
H	-6.0351	-1.9607	3.2236
H	-6.4098	-1.7773	0.7691
H	-4.4839	-1.4827	-0.7580
H	-1.7974	-1.5401	2.5969
H	-3.7213	-1.8455	4.1277

TS5
Gasphase Energy: -638.4360
Solvation Phase Energy: -638.4494
Zero Point Energy: 78.72 kcal/mol
Imaginary Frequency: -79.05 cm-1
Coordinates:

Ir	-0.1105	0.0187	0.0172
O	-0.2413	-0.0248	2.0596
O	1.8631	-0.1772	0.1041
C	2.5693	-0.2679	-0.9659
C	2.1638	-0.2511	-2.2952
C	0.8408	-0.0731	-2.7332
O	-0.1964	0.0690	-2.0156
H	0.6600	-0.0342	-3.8132
H	2.9350	-0.3453	-3.0509
H	3.6373	-0.3621	-0.7473

H	-0.0607	-1.5436	-0.0236
O	-0.7155	2.1235	0.0079
C	-0.8999	2.7744	1.0834
C	-0.4887	0.9990	2.7847
C	-0.7771	2.3122	2.4021
H	-1.2019	3.8252	0.9559
H	-0.4838	0.7832	3.8597
H	-0.9644	3.0243	3.1985

TS6
Gasphase Energy: -1026.7167
Solvation Phase Energy: -1026.7227
Zero Point Energy: 200.37 kcal/mol
Imaginary Frequency: -447.79 cm-1
Coordinates:

Ir	0.0601	0.0834	0.0255
O	-0.1953	0.1427	2.0566
O	2.2339	0.0325	0.3782
C	3.0283	0.0632	-0.6040
C	2.7243	0.1087	-1.9804
C	1.4552	0.0994	-2.5631
O	0.2999	0.0315	-2.0183
H	1.4182	0.1337	-3.6592
H	3.5664	0.1533	-2.6632
H	4.0996	0.0479	-0.3490
O	0.3434	2.0980	-0.1710
C	0.3155	2.8633	0.8477
C	-0.1136	1.2445	2.6947
C	0.1134	2.5296	2.1924
H	0.4736	3.9221	0.6106
H	-0.2476	1.1432	3.7781
H	0.1373	3.3420	2.9103
C	0.0142	-2.3075	0.1415
H	1.0142	-2.0010	0.4610
H	-0.3498	-2.9128	0.9719
C	0.1098	-3.1199	-1.1557
H	-0.8671	-3.5562	-1.4002
H	0.3734	-2.4577	-1.9839
C	-1.7720	-1.4319	0.1468
C	-1.9740	-0.0443	-0.2652
H	-2.1070	-2.2129	-0.5306
H	-2.2441	0.1205	-1.3086
H	-2.5412	0.5775	0.4295
H	-2.0095	-1.6339	1.1870
C	3.0324	-6.2985	-0.7686

C	3.4191	-5.0399	-1.2364
C	2.4755	-4.0197	-1.3693
C	1.1300	-4.2378	-1.0374
C	0.7545	-5.5057	-0.5701
C	1.6953	-6.5289	-0.4360
H	3.7657	-7.0939	-0.6681
H	4.4562	-4.8536	-1.5028
H	2.7796	-3.0422	-1.7373
H	-0.2867	-5.6942	-0.3160
H	1.3836	-7.5061	-0.0765

TS7
Gasphase Energy: -1026.7149
Solvation Phase Energy: -1026.7227
Zero Point Energy: 196.96 kcal/mol
Imaginary Frequency: -447.71 cm-1
Coordinates:

Ir	0.0252	0.0522	0.0708
O	-0.1364	0.5003	2.1462
C	0.8956	0.5212	2.8847
C	2.2334	0.2881	2.5345
C	2.7079	-0.0437	1.2646
O	2.0632	-0.2188	0.1762
H	3.7896	-0.1885	1.1589
H	2.9709	0.3714	3.3252
H	0.3810	1.3126	-2.1327
O	-2.0112	0.3352	-0.0244
O	0.4286	2.1950	0.0196
C	-0.5353	3.0181	0.0207
C	-2.5295	1.5027	-0.0188
C	-1.9157	2.7572	0.0011
H	-0.2426	4.0785	0.0304
H	-3.6260	1.4899	-0.0367
H	-2.5753	3.6182	0.0008
C	-0.3706	-1.8922	0.6409
H	-0.7920	0.0586	-2.5788
C	1.3095	-0.5119	-2.8443
H	1.0843	-1.5848	-2.8885
H	2.2321	-0.4059	-2.2667
H	-1.4133	-2.0187	0.9332
H	0.1884	-3.8630	1.1489
C	0.4948	-2.9018	0.7395
H	1.5321	-2.8119	0.4282
H	0.6984	0.7597	3.9388
H	-0.0872	-1.0266	-1.0550

C	0.1828	0.2396	-2.1171
C	1.8330	1.0729	-6.8441
C	0.9843	-0.0151	-6.6260
C	0.8239	-0.5315	-5.3383
C	1.5074	0.0260	-4.2485
C	2.3570	1.1180	-4.4813
C	2.5198	1.6383	-5.7664
H	1.9615	1.4742	-7.8455
H	0.4497	-0.4647	-7.4586
H	0.1651	-1.3820	-5.1759
H	2.8983	1.5581	-3.6465
H	3.1866	2.4814	-5.9272